Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Computationally efficient dielectric calculations of molecular crystals KATHLEEN SCHWARZ, Cornell University Department of Chemistry and Chemical Biology, T.A. ARIAS, Cornell University Department of Physics —
The dielectric response is a key quantity for electronic materials such as organic semiconductors. Calculations of the dielectric response for molecular crystals are currently either expensive, or rely on extreme simplifications such as multipole expansions. We present an alternate approach using an analogue of the Clausius-Mossotti equation, which constructs the crystal's dielectric response from an eigenvalue decomposition of the molecular dielectric response. This method can be used to examine the effects of defects and surfaces on the dielectric properties of molecular crystals.

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Date submitted: 09 Nov 2012 Electronic form version 1.4